

1,3-Benzodioxole-5-methanol
495-76-1 | DTXSID3060089

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.45

Global applicability domain: Inside

Local applicability domain index: 5.40e-01

Confidence level: 7.86e-01

Nearest Neighbors from the Training Set

Image not found

2-Isopropyl-6-methyl-4-pyrimidone

Measured: 1.82

Predicted: 2.23

Image not found

2,2-Dimethylpropane-1,3-diol

Measured: 4.68

Predicted: 4.44

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1,1'-Oxybis-2-propanol

Measured: 4.57

Predicted: 3.83

Image not found

Paraldehyde

Measured: 3.02

Predicted: 2.77

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2,2-Bis(bromomethyl)-1,3-propanediol

Measured: 4.79

Predicted: 3.35